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Comparison of modeling approaches to quantify residue architecture effects on soil temperature and water

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Abstract

RZ-SHAW is a hybrid model, comprised of modules from the Simultaneous Heat and Water (SHAW) model integrated into the Root Zone Water Quality Model (RZWQM) that allows more detailed simulation of different residue types and architectures that affect heat and water transfer at the soil surface. RZ-SHAW allows different methods of surface energy flux evaluation to be used: (1) the SHAW module, where evapotranspiration (ET) and soil heat flux are computed in concert with a detailed surface energy balance; (2) the Shuttleworth–Wallace (S–W) module for ET in which soil surface temperature is assumed equal air temperature; and (3) the PENFLUX module, which uses a Penman transformation for a soil slab under incomplete residue cover. The objective of this study was to compare the predictive accuracy of the three RZ-SHAW modules to simulate effects of residue architecture on net radiation, soil temperature, and water dynamics near the soil surface. The model was tested in Akron, Colorado in a wheat residue-covered (both standing and flat) no-till (NT) plot, and a reduced till (RT) plot where wheat residue was incorporated into the soil. Temperature difference between the soil surface and ambient air frequently exceeded 17 °C under RT and NT conditions, invalidating the isothermal assumption employed in the S–W module. The S–W module overestimated net radiation (R_n) by an average of 69 Wm^{-2} and underestimated the 3-cm soil temperature (T_{s3}) by 2.7 °C for the RT plot, attributed to consequences of the isothermal assumption. Both SHAW and PENFLUX modules overestimated midday T_{s3} for RT conditions but underestimated T_{s3} for NT conditions. Better performances of the SHAW and PENFLUX surface energy evaluations are to be expected as both approaches are more detailed and consider a more discretized domain than the S–W module. PENFLUX simulated net radiation slightly better than the SHAW module for both plots, while T_{s3} was simulated the best by SHAW, with a mean bias error of +0.1 °C for NT and +2.7 °C for RT. Simulation results for soil water content in the surface 30 cm (θ_{v30}) were mixed. The NT conditions were simulated best by SHAW, with mean bias error for θ_{v30} within 0.006 m^3 m^{-3}; RT conditions were simulated best by the PENFLUX module, which was within 0.010 m^3 m^{-3}.

Keywords: Energy balance; Penman flux module (PENFLUX); Root Zone Water Quality Model (RZWQM); Simultaneous Heat and Water (SHAW) Model; Shuttleworth–Wallace

1. Introduction

Residue and tillage management are important tools for conserving soil and water resources. Cool and wet soil

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conditions are known to be associated with reduced tillage and surface retention of residues (Allmaras et al., 1977). Increased soil water storage with higher quantities of residue loading was attributed to improved infiltration and reduced evaporation (Doran et al., 1984). Residue management affects the thermal dynamics of evaporative surfaces, thus modifying energy balance components, including longwave radiation and partitioning of absorbed radiation to sensible, latent, and soil heat fluxes. Residue architecture (dimension, frequency, and orientation of residue elements) modifies radiative and advective exchange processes between soil and atmosphere (Raupach, 1992; Flerchinger et al., 2003; Sauer and Norman, 1995). Knowledge of plant residue effects on the soil energy balance can guide farm and regional assessment of residue management alternatives for: soil, water, and nutrient conservation; pest management; and plant development processes (Van Doren and Allmaras, 1978). Accurate simulation of the energy exchange processes in the soil–residue–atmosphere can enhance understanding of residue type and architecture effects (Aiken et al., 1997).

Researchers have simulated the effects of residue on soil temperature and water using computer models for over two decades. Bristow et al. (1986) developed one of the first detailed simulation models of heat and water transfer through surface residues. Lascano et al. (1987) and Lascano and Baumhardt (1996) evaluated the ENWATBAL model for simulating evaporation from sparse crops and residues. Flerchinger and Saxton (1989) developed and applied the Simultaneous Heat and Water (SHAW) model to simulate the effects of surface residues on soil freezing. Aiken et al. (1997) evaluated a Penman-type energy balance module, PENFLUX, for simulating the surface energy balance with residues present. More recently, Flerchinger et al. (2003) simulated the effects of standing versus flat residue on the soil surface using the SHAW model.

The Root Zone Water Quality Model (RZWQM) is a comprehensive agricultural system model for predicting soil physical and chemical processes and crop growth. Soil water and heat transfer, evapotranspiration, and biomass accumulation are essential components of the model (Ahuja et al., 2000a). The model was designed to simulate carbon–nitrogen cycles, as well as water and fertilizer management. The Green–Ampt equation is used for water infiltration during rainfall irrigation events, and the Richards' equation is used for water redistribution between events (Ahuja et al., 2000b).

Currently, RZWQM uses a modified two-layer approach (Shuttleworth and Wallace, 1985; S–W) to calculate the surface energy balance equation. Penman (1948) partitioned net radiative energy into sensible and latent heat for land surfaces assuming the surface as a single source/sink for heat fluxes. This concept has been applied to uniform crops with the canopy regarded as a single uniform surface or a single big-leaf, as in the Penman–Monteith (P–M) evaporation model (Monteith, 1965). However, fields with sparse canopy do not satisfy the big-leaf assumption as sources/sinks of fluxes may occur at significantly separated surfaces, i.e., at the canopy and the soil surface. To account for this, the single-layer P–M ET model has been extended to two layers, the S–W model (Shuttleworth and Wallace, 1985). Farahani and Bausch (1995) and Farahani and Ahuja (1996) extended the S–W model to describe ET process under no-till or minimum-till practices that leave a portion of crop residue on the soil surface. The extended S–W model attempts to synthesize previous efforts and findings in conjunction with the double-layer energy combination approach. It explicitly defines a partially covered soil and predicts evaporation from bare soil fraction of the substrate, the residue covered fraction of the substrate, and transpiration from canopy. Based on this approach, net radiation, sensible heat, and latent heat fluxes are calculated. However, in RZWQM the soil heat flux is considered zero. Therefore, the boundary conditions for the heat transfer in the soil are affected; the model assumes the upper boundary condition of the soil surface to equal the ambient air temperature, e.g., isothermal soil surface—ambient conditions.

To overcome this limitation at the boundary surface, a hybrid model (RZ-SHAW, an integration of RZWQM and a mechanistic soil heat and water model, SHAW) was developed to improve soil surface temperature simulation and soil temperature simulation in RZWQM (Flerchinger et al., 2000). SHAW includes detailed provisions for heat and water transfer through a plant canopy, a complete energy balance for multiple layers of snowpack, and heat and water transfer within a residue layer. Because of its layered structure, SHAW can simulate temperature in the plant canopy, surface residue, and soil surface and has been critically validated against experimental data (Flerchinger and Saxton, 1989; Sharratt and Flerchinger, 1995; Flerchinger et al., 2003). Soil heat flux and surface temperatures are determined in concert with the energy balance routines.

However, the SHAW module can be computationally expensive; a simpler and computationally efficient Penman-type module (PENFLUX, Aiken et al., 1997) option was added to RZ-SHAW for non-winter conditions. PENFLUX solves for surface temperatures of a soil slab, a single flat residue layer (adjusting for aerodynamic resistances of standing residue stems), and a plant canopy layer; therefore, expanding the two-layer model of S–W to three while giving explicit consideration to temperature gradients in the soil–residue–atmosphere continuum. It provides surface boundary conditions for simulations of energy transfer in a one-dimensional soil profile. PENFLUX simplifies iterative solutions by simplifying radiation, convective, and soil heat algorithms. The calculated soil heat flux value is used as the upper boundary condition in the soil heat transfer equations of RZWQM.

RZ-SHAW allows three different levels of complexity for evaluating the surface energy balance and therefore upper boundary condition for the soil heat equation, i.e., S–W, SHAW, and PENFLUX. The objective of this study was to evaluate RZ-SHAW under the three different options for surface energy balance by comparing simulated net radiation, soil temperatures, and water contents with experimental results of two field conditions in Akron, Colorado: (1) a wheat residue-covered (both standing and flat, NT) plot; and (2) a reduced till (RT) plot where wheat residue was incorporated into the soil. Results of this study elucidate the detail needed to adequately capture the influence of residue characteristics on soil temperature and water dynamics.

2. Materials and methods

Radiation and thermal and soil water dynamics were quantified during the 14-month fallow period between 1995 wheat harvest and 1996 planting at the Central Great Plains Research Station, Akron, Colorado. Wheat stubble in field plots (9.1 m × 30.5 m, oriented E–W) was managed as no-till (NT) or as stubble-mulch reduced till (RT) systems. The study plots were located on a Weld silt loam soil (fine montmorillonitic, mesic Aridic Paleustoll). Weather data collected on site included hourly shortwave irradiance (LiCor 200 pyranometer, Lincoln, NE), ambient temperature and relative humidity at 2 m above the soil surface (Vaisala HMP35A, Woburn, MA.), and horizontal wind velocity and direction (Met One 034 A, Grants Pass, OR) at 2 m height. Precipitation observations were collected from a shielded, weighing precipitation gauge.

Instrumentation for each experimental site included a net radiometer (REBS Q*7.1, Seattle, WA) and an inverted Epply type pyranometer, quantifying reflected shortwave radiation, installed 1.5 m above the soil surface; a similar pyranometer quantified incoming shortwave radiation. Net shortwave radiation was calculated as the difference between incoming and reflected irradiance. Thermocouple thermometers (24 ga., type T) measured soil temperature at 3, 7, 15 and 25 cm depths. A bare-wire surface thermocouple was embedded in the upper 0.5-cm soil layer and secured by staple. Similarly, a thermocouple was inserted 10 mm, axially, into an intact wheat stem lying on the soil surface. Fine-wire thermocouples sensed ambient temperatures 3 and 30 cm above the soil surface. A needle anemometer (NA-27, Soiltronics, Burlington, WA) oriented vertically, quantified horizontal wind speed 3 cm above the soil surface (Bland et al., 1995). Pyranometers and anemometers were calibrated before and after deployment against instruments reserved for use as calibration standards. A data logger (CR 21X, Campbell Scientific, Logan, UT) sampled sensor output at 60 s intervals and recorded average values at 1-h intervals. Soil water content (0–30 cm depth interval) was measured periodically with duplicate sets of vertically installed 30-cm TDR rods read with a Trase 6050X1 instrument (SoilMoisture Equipment Corporation, Santa Barbara, CA). Sensors were removed and replaced to accommodate tillage operations under RT management.

Surface residue cover was quantified using a 200-point line intercept method (Morrison et al., 1993) for the NT plot; standing stem architecture (height, frequency and diameter) was quantified by sampling one meter of row. Standing stem observations were used to estimate the stem area index (the projected area of standing stems onto a vertical plane for a unit of ground area, $m^2\ m^{-2}$). A summary of residue cover for the NT plot and characteristics and soil properties for both plots are given in Tables 1 and 2, respectively.

Soil energy and water balances were simulated from May 6, 1996 to September 10, 1996 using the SHAW, S–W, and PENFLUX modules, parameterized for each plot. The model was initialized with measured soil temperature and water content on May 6 for each module and was driven with weather observations of air temperature, relative humidity, wind speed, solar radiation and precipitation that are required for each of the modules. Site conditions input to the modules included residue parameters listed in Table 1 for the NT plot, and soil parameters in Table 2. The RT plot was simulated as a bare soil surface.

Table 1
Residue characteristics for no-till (NT) field conditions

Flat residue loading (kg ha^{-1})	3.3
Age of residue (days)	100
Height of flat residue mass (cm)	1.13
Standing residue mass (kg ha^{-1})	1.08
Standing stem area index ($m^2\ m^{-2}$)	0.19
Stem height (cm)	23.2

Table 2
Soil layering and physical properties of weld silt loam (fine montmorillonitic, mesic Aridic Paleustoll)

Horizon	Depth (cm)	Bulk density (g cm^{-3})	Porosity	Sand (%)	Silt (%)	Clay (%)
Ap	0–10	1.35	0.49	30	50	20
Bt1	10–20	1.32	0.51	30	40	30
Bt2	20–35	1.32	0.51	25	40	35
Bk	35–60	1.32	0.51	40	40	20
Ck	60–140	1.32	0.51	45	45	10

The model simulation results were compared with measured net radiation (R_n), 3-cm soil temperature (T_{s3}) and water content in the surface 30-cm interval (θ_{v30}) for different time periods during the study. The simulated and measured data were analyzed, and the mean bias error (MBE), root mean square error (RMSE), and the model efficiency (ME) of the simulated results were calculated (Green and Stephen-

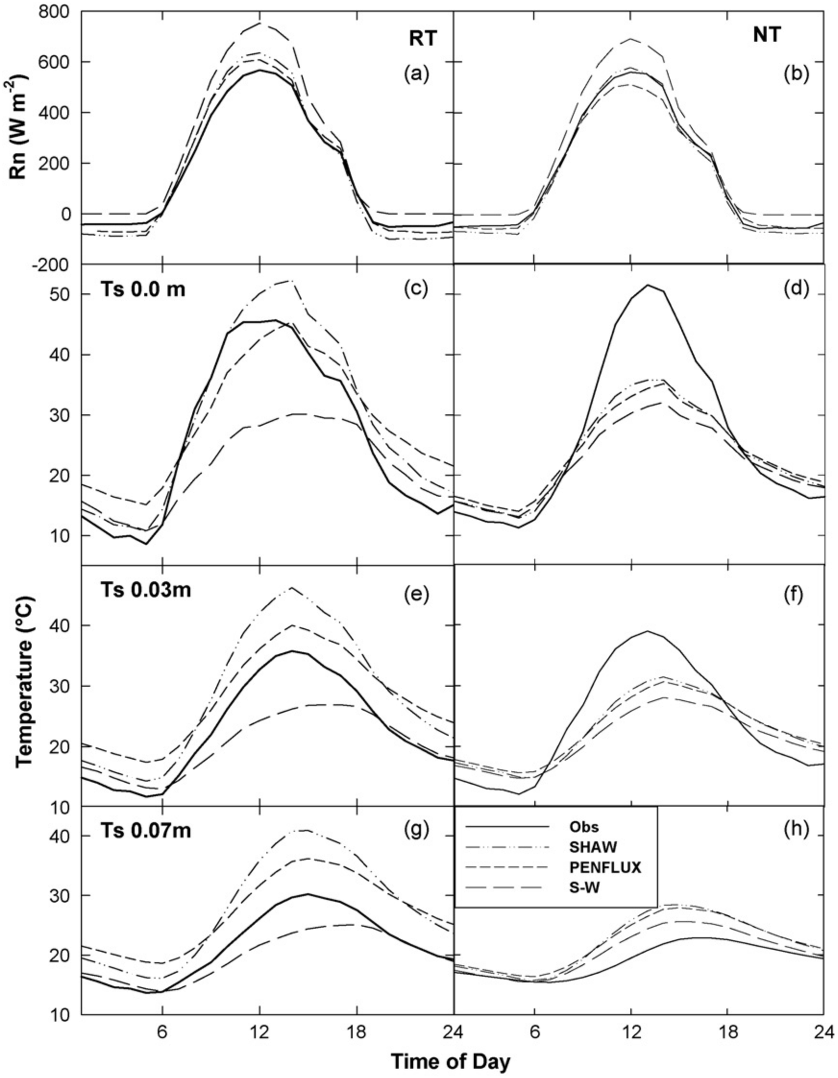

Fig. 1. Measured and simulated results of net radiation, R_n (a and b), and soil temperatures, T_s, at surface depth (c and d), at 3-cm depth (e and f) and at 7-cm depth (g and h) under RT and NT conditions, respectively, using RZ-SHAW modules SHAW, S–W, and PENFLUX for May 15, 1996 (DOY 136).

Table 3
Description and definition of model performance measures (Green and Stephenson, 1986)

Measure	Description	Mathematical definition
MBE	Mean bias error of model predictions compared to observed values	$\frac{1}{N}\sum_{i=1}^{N}(\hat{Y}_i - Y_i)$
RMSE	Root mean square error between model predictions and observed values	$\left[\frac{1}{N}\sum_{i=1}^{N}(\hat{Y}_i - Y_i)^2\right]^{1/2}$
ME	Model efficiency, i.e., variation in measured values accounted for by model	$1 - \frac{\sum_{i=1}^{N}(Y_i-\hat{Y}_i)^2}{\sum_{i=1}^{N}(Y_i-\bar{Y}_i)^2}$

$\hat{Y}_i$, simulated values; Y_i, observed values; $\bar{Y}$, mean of observed *values*; N, number of observations.

son, 1986). Descriptions of the statistical analyses are summarized in Table 3. Detailed analysis of predictive accuracy for a 5-day period with near-clear sky conditions (DOY 136–140) included linear regressions between simulated values for a given simulation module against field observations. To assess diel (daily) patterns in predictive error, observed values were subtracted from values calculated by a simulation model for each hourly time interval within an evaluation period. Thus, a positive predictive error corresponded to positive bias. Mean deviations were computed for each hour of an evaluation period.

3. Results

Residue and tillage effects on radiation and near-surface temperatures are depicted in Fig. 1 for day of year (DOY) 136, a nearly clear day with dry surface soil conditions. Total net irradiance values (R_n) were virtually identical for both NT and RT conditions (Fig. 1(a and b)). Surface temperatures deviated from ambient during daytime, but were similar at night. Surface soil warming occurred earlier under RT conditions; however, maximum surface soil temperature occurred under NT conditions (Fig. 1(c and d)). Although morning soil temperatures increased at the 3-cm layer earlier under NT conditions (Fig. 1(e and f)), the 7-cm soil temperature increased more rapidly under RT conditions (Fig. 1(g and h)).

The predictive accuracy of simulation results for the three modules are compared with field observations on DOY 136 for R_n, T_{s0}, T_{s3}, and T_{s7} in Fig. 1. Regression and RMSE analyses for these parameters are reported for the DOY 136–140 period, a sequence of early summer days with nearly clear sky and dry surface soil conditions, in Table 4. Diel variation in simulated soil temperature bias is evaluated in Fig. 2 for this same period. Mean bias error (MBE), model efficiency (ME) and root mean square error (RMSE) for R_n, T_{s3}, and θ_{v30} are reported for a 125-day summer period in Table 5.

Values for R_n, calculated with the S–W module, exhibited positive bias (predicted values exceed

Table 4
Regression analysis for predictive accuracy of three energy balance modules of RZ-SHAW simulation, relative to field measurements DOY 136–140

RZ-SHAW module[a]	NT				RT			
	Intercept	Slope	r^2	RMSE	Intercept	Slope	r^2	RMSE
Net radiation (Wm^{-2})								
SHAW	−27.5[b]	1.06[b]	0.993	20.5	−37.5[b]	1.18[b]	0.992	24.8
S–W	38.6[b]	1.12[b]	0.988	28.7	40.1[b]	1.19[b]	0.990	28.2
PENFLUX	4.1	1.02	0.987	25.3	−15.2[b]	1.12[b]	0.990	26.6
Soil temperature 0-cm depth (°C)								
SHAW	9.44[b]	0.54[b]	0.933	1.94	2.88[b]	1.06[b]	0.967	2.49
S–W	11.29[b]	0.41[b]	0.926	1.55	8.83[b]	0.49[b]	0.817	2.92
PENFLUX	11.57[b]	0.46[b]	0.937	1.59	12.17[b]	0.69[b]	0.922	2.54
Soil temperature 3-cm depth (°C)								
SHAW	9.31[b]	0.54[b]	0.861	1.97	−2.05[b]	1.36	0.974	1.60
S–W	11.23[b]	0.44[b]	0.827	1.68	7.10[b]	0.59[b]	0.779	2.29
PENFLUX	11.4[b]	0.49[b]	0.846	1.77	8.11[b]	0.90[b]	0.949	1.53
Soil temperature 7-cm depth (°C)								
SHAW	−8.49[b]	1.56[b]	0.786	1.89	−7.18[b]	1.63[b]	0.967	1.43
S–W	−3.87[b]	1.25[b]	0.853	1.21	4.77[b]	0.71[b]	0.778	1.79
PENFLUX	7.44[b]	0.70[b]	0.833	0.73	4.31[b]	1.09[b]	0.941	1.30

[a] SHAW is a module derived from the Simultaneous Heat and Water model; S–W is based on Shuttleworth–Wallace equation; and PENFLUX is a Penman transformation for incomplete residue cover.
[b] Regression coefficients for intercept or slope differ ($p < 0.05$) from 0 or 1, respectively.

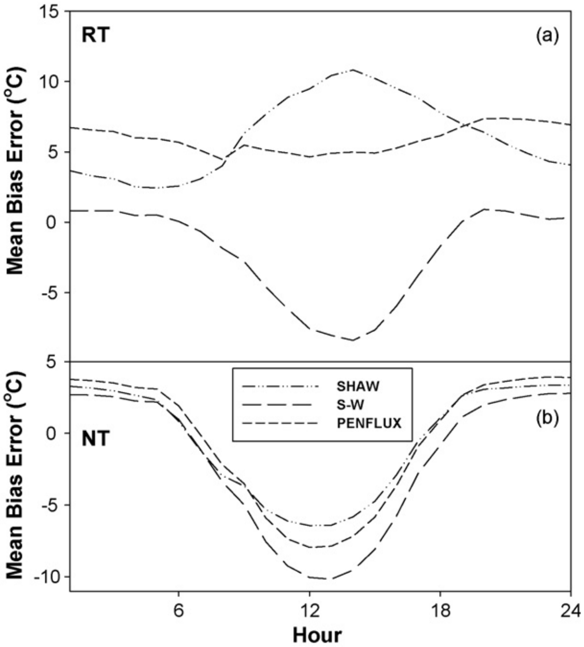

Fig. 2. Mean bias error (hourly basis) for predictive accuracy of soil temperature (3-cm depth) using RZ-SHAW modules (a) SHAW, (b) S–W, and (c) PENFLUX for May 15–20, 1996 (DOY 136–141).

observed values). This bias was proportionate to irradiance values under both RT and NT conditions, as suggested by the slope of the regression line being significantly greater than 1.0 (Table 4). Net radiation values calculated with the SHAW energy balance module resulted in a negative nocturnal bias, as suggested by the negative intercepts in Table 4, and positive diurnal bias relative to field observations, which was stronger for RT (Fig. 1a) than for NT (Fig. 1b) conditions, as suggested by the larger regression slope for RT compared to NT (1.18 versus 1.06 in Table 4). These trends can also be seen in Figs. 3 and 4. Simulation values of R_n with the PENFLUX energy balance module were similar to that of the SHAW module for RT conditions (Fig. 3). However, the slope and intercept (1.02 and 4.1 °C, Table 4) for the PENFLUX NT simulation are not significantly different from 1.0 and 0.0 °C, indicating that PENFLUX did not have a significant bias in net radiation for NT conditions. Predictive accuracy for R_n was greatest for the PENFLUX module, which exhibited a slight positive mid-day bias, and least for the S–W module, exhibiting positive bias day and night. A negative bias in R_n at night resulted from both PENFLUX and SHAW modules.

Surface soil temperature is set equal to ambient temperature in the S–W module. This isothermal assumption ($T_{s0} = T_a$) resulted in least bias at night (Figs. 1 and 2), but in a negative bias for T_{s0} (both NT and RT condition), which was greatest around midday when net radiation was highest (Fig. 2). As a consequence, offsetting biases in slope and intercept (0.41 and +11.29 °C for NT in Table 4) resulted for T_{s0} values calculated by the S–W module during the DOY 136–140 period for both NT and RT conditions. This negative daytime bias, attributed to the isothermal assumption used in the S–W module, persisted throughout the season for both RT and NT conditions (Figs. 5 and 6).

The SHAW and PENFLUX modules include explicit calculations of surface temperature and gradients

Table 5
Performance measures for predictive accuracy of three energy balance modules of RZ-SHAW simulation, relative to field measurements

RZ-SHAW module[a]	NT			RT		
	MBE	RMSE	ME	MBE	RMSE	ME
Net radiation DOY 127–250 (Wm^{-2})						
SHAW	−40.3	52.1	0.94	0.2	62.2	0.92
S–W	31.6	56.1	0.94	68.9	99.5	0.81
PENFLUX	−25.5	47.0	0.96	5.0	60.6	0.93
3-cm soil temperature DOY 127–250 (°C)						
SHAW	0.11	3.2	0.84	2.7	4.0	0.69
S–W	−0.94	5.2	0.57	−2.7	4.4	0.64
PENFLUX	0.44	6.2	0.40	4.2	4.8	0.57
30-cm surface soil water content DOY 150–248 (°C)						
SHAW	−0.006	0.018	0.44	−0.044	0.050	−1.88
S–W	−0.033	0.039	−1.63	−0.033	0.040	−0.91
PENFLUX	−0.014	0.022	0.13	0.010	0.027	0.14

[a] SHAW is a module derived from the Simultaneous Heat and Water model; S–W is based on Shuttleworth–Wallace equation; and PENFLUX is a Penman transformation for incomplete residue cover.

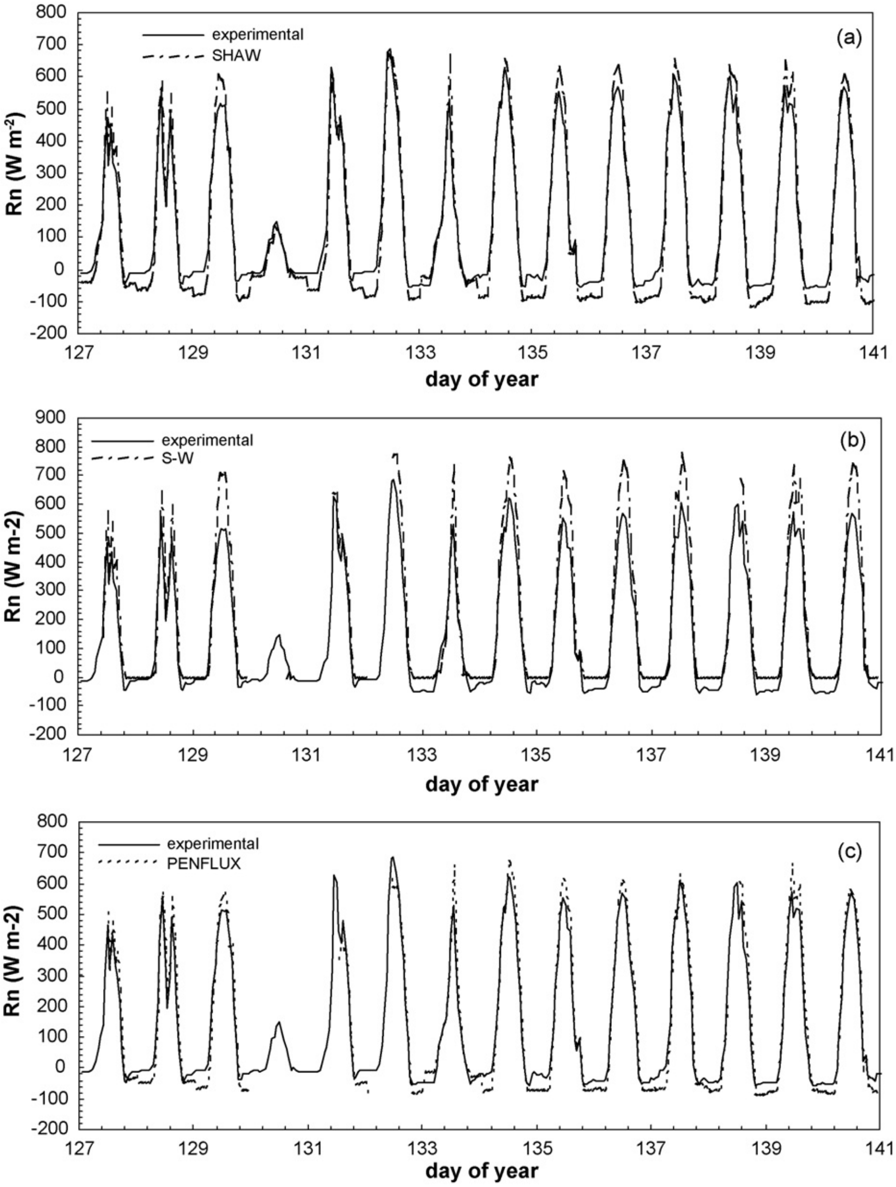

Fig. 3. Measured and simulated results of net radiation, R_n, under RT conditions using RZ-SHAW modules (a) SHAW, (b) S–W, and (c) PENFLUX for May 6–20, 1996 (DOY 127–141).

against ambient conditions. The predictive accuracy of these two modules differed for NT and RT conditions. Calculated values for T_{s0} from both modules under NT conditions resulted in a negative bias (Fig. 1d) during daytime and a slight positive bias at night. Both timing and amplitude of simulated soil temperature dynamics at 3 and 7 cm failed to match field observations (Fig. 1(f and h)). This shift in bias during the day was evident for T_{s3} during the DOY 136–140 interval (Fig. 2b, 6) and confirmed by offsetting biases in slope (less than 1.0) and intercept (greater then 0.0 °C) of the regression line between simulated and observed values in Table 4. However, MBE for T_{s3} was only 3% of RMSE for values calculated by SHAW when averaged over the summer period (Table 5); ME was largest for SHAW values as well.

Under RT conditions, values simulated for T_{s0} with the SHAW module corresponded more closely with field observations (Fig. 1c) than for NT (Fig. 1d) conditions and resulted in the least bias in predictive accuracy for T_{s0} during the DOY 136–140 interval, with an intercept of 2.88 °C and slope of 1.06 (Table 4).

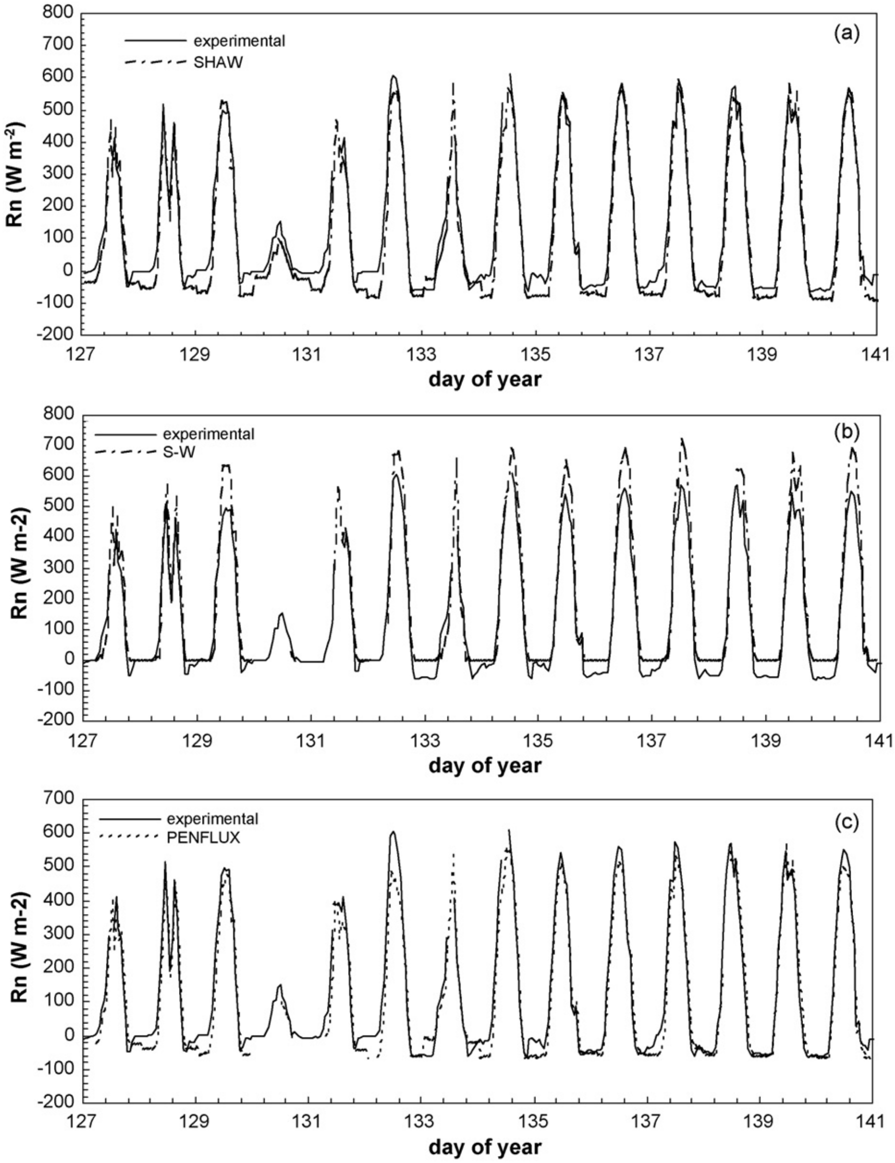

Fig. 4. Measured and simulated results of net radiation, R_n, under NT conditions using RZ-SHAW modules (a) SHAW, (b) S–W, and (c) PENFLUX for May 6–20, 1996 (DOY 127–141).

SHAW simulation of warming of 3 and 7-cm soil layers for RT conditions (Fig. 1(e and g)) corresponded to field observations in timing of diel maxima but not in amplitude. Increasing divergence from 0.0 and 1.0 in the intercept and slope between T_{s0}, T_{s3} and T_{s7} indicates errors in simulation of heat transfer into the soil. Daytime maxima of T_{s0} for RT conditions were simulated with greater accuracy with the PENFLUX module. Temperature dynamics of T_{s3} and T_{s7} were also more closely simulated by the PENFLUX module, though a substantial offset reflected a persistent positive bias. The smallest bias in diel variation of T_{s3} (Fig. 2a) and T_{s7} (data not shown) values was simulated by the PENFLUX module, though a constant positive offset was evident.

Soil water content (0–30-cm interval) was calculated by RZ-SHAW using energy-limiting evaporation rates enforced as boundary conditions that were calculated by the energy balance modules. Simulated and observed θ_{v30} are shown for RT (Fig. 7) and NT (Fig. 8) conditions. Predictive accuracy using PENFLUX potential evaporation values was equal to that of the SHAW module for NT conditions and greatest among the modules for RT conditions. A persistent negative

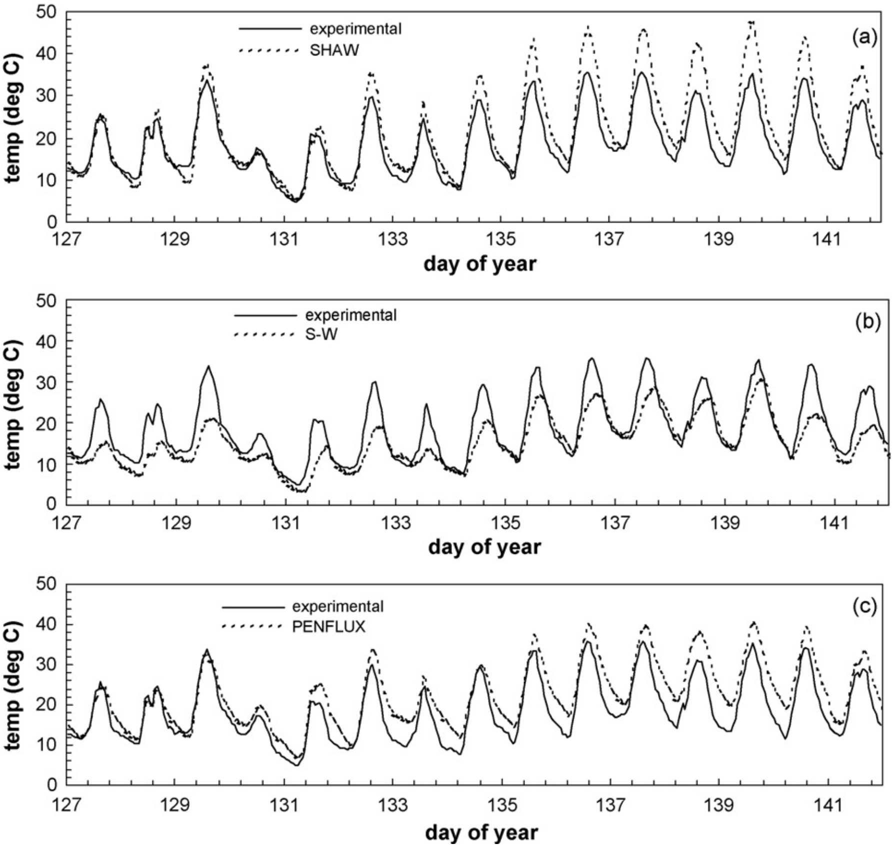

Fig. 5. Measured and simulated results of soil temperature (3-cm depth, RT conditions) using RZ-SHAW modules (a) SHAW, (b) S–W, and (c) PENFLUX for May 6–20, 1996 (DOY 127–141).

bias reduced accuracy of soil water calculations for the S–W module, under both RT and NT conditions.

4. Discussion

The isothermal assumption of the S–W module ($T_{s0} = T_a$) appeared appropriate at night for surface soil and residue temperatures. Predictive accuracy for the S–W module was reasonably good from 18:00 to 6:00 when sensible heat flux is negligible. The negative bias of SHAW and PENFLUX modules may result from parameterization errors in soil thermal properties or in long-wave atmospheric emittance. During daytime, persistent negative bias in S–W value for T_{s0} (as well as R_n) indicate the isothermal assumption was not warranted for this dry semi-arid climate where the soil can warm considerably higher than air temperature. Maximum difference between surface and atmosphere temperature gradients exceeded 20 °C for both RT and NT conditions. The S–W module may perform better under more humid climates with wetter surface soil conditions, however Bristow (1988) reported similar temperature gradients for a soil in sub-tropical conditions.

Soil water dynamics calculated with S–W boundary conditions (e.g. potential evapotranspiration) exhibited a persistent negative bias. This bias is attributed to error propagated from a positive bias in R_n, which appears to be associated with the isothermal assumption. The persistent negative bias in θ_{v30} calculated with the S–W module is attributed to the positive bias in R_n and simplifying assumption that $G = 0$ which would tend to a positive bias in evaporative flux. Values simulated for evaporative flux with the S–W module would be reduced if G were calculated from the change in heat storage associated with soil temperature dynamics (similar to the approach used in PENFLUX), and re-evaluating the empirical proportionality in R_n due to non-isothermal conditions.

Error in surface temperature propagates to energy balance components of net longwave radiation (R_{nl}), sensible heat flux (H), latent heat flux (LE) and soil heat flux (G). For example, a negative bias in T_{s0} of 20 °C would propagate to a positive bias of 124 Wm^{-2} (e.g.,

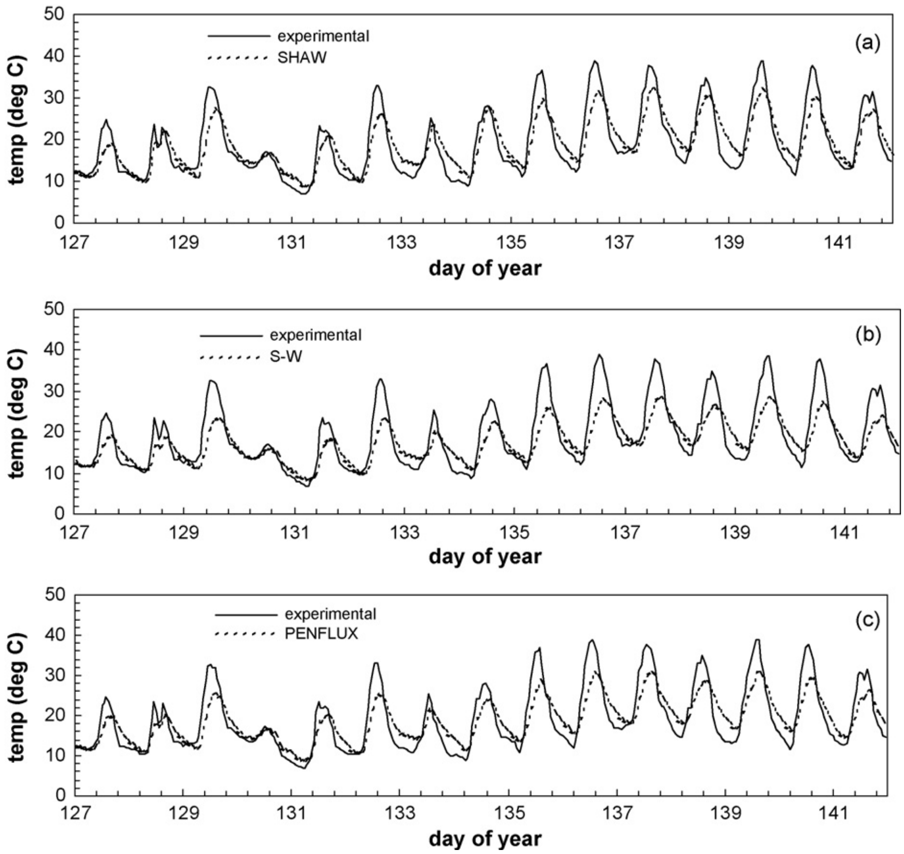

Fig. 6. Measured and simulated results of soil temperature (3-cm depth, NT conditions) using RZ-SHAW modules (a) SHAW, (b) S–W, and (c) PENFLUX for May 6–20, 1996 (DOY 127–141).

$\varepsilon\sigma[T_1^4 - T_2^4] = 0.97 \times 5.76 \times 10^{-8}\ \mathrm{Wm^{-2}\ K^{-4}}$ $[(300\ \mathrm{K})^4 - (280\ \mathrm{K})^4] = 124\ \mathrm{Wm^{-2}}$) in R_{nl} under dry soil conditions. Under radiative loading, the isothermal assumption can be expected to result in error in surface temperature T_{s0}. Propagation of error to derived parameters such as R_{nl} and G can be significant. The excessive R_n simulated by the S–W module is attributed to the isothermal assumption and propagation of bias in surface soil temperatures to R_{nl}.

Both SHAW and PENFLUX modules consider surface–atmosphere temperature gradients and are therefore applicable to a broader range of climatic conditions than the S–W module. The SHAW and PENFLUX modules mimic the diel amplitude in surface temperatures observed for RT conditions, but display a positive bias in maximum daily T_{s3}. Neither of the modules captured the observed diel amplitude for the NT conditions, and both modules give negative bias for maximum daily T_{s3} under NT conditions during periods of radiative loading. The observed mean bias error could result from model mis-specification of surface crop residue effects on radiation transmission, absorbance, and heat storage by standing stems and on convective transport within the residue sub-layer. For example, the sheltering effects of standing wheat stems (Aiken et al., 2003) likely reduced convective dissipation of heat in the residue sub-layer and led to the warmer surface conditions. The persistent positive bias of PENFLUX calculation of T_{s3} under RT conditions is attributed to cumulative error in simulating heat dissipation associated with the soil slab approximation. The shifting bias in T_{s3} with presence and absence of crop residue indicates module mis-specification of near-surface energy exchange processes for both SHAW and PENFLUX modules.

The SHAW and PENFLUX modules exhibited similar predictive accuracy for R_n and T_{s3} but not for soil water. Predictive accuracy for soil water under NT was good for both modules. Under RT conditions, predictive accuracy was retained for the PENFLUX module, but SHAW boundary conditions resulted in a negative bias for soil water. The energy balance modules affect calculations of the soil water balance by the evaporative flux term (LE). Each energy balance

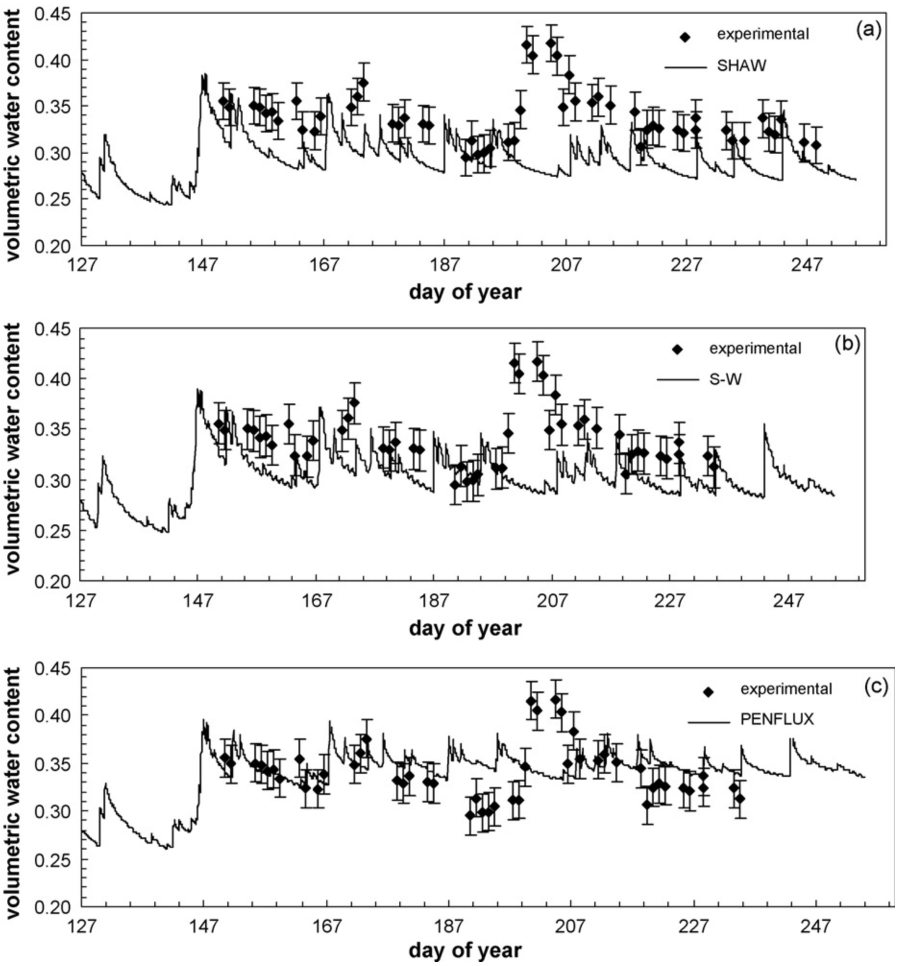

Fig. 7. Measured and simulated results of soil water content (0–30-cm interval, RT conditions) using RZ-SHAW modules (a) SHAW, (b) S–W, and (c) PENFLUX for May 6–September 10, 1996 (DOY 140–254).

module passes an evaporation rate (mm h^{-1}) to the soil water balance equation, thereby establishing a limiting rate for evaporation. Thus, errors in surface energy balance modules affecting LE will propagate to calculation of soil water dynamics in surface soil layers during stage I evaporation. The generally drier soil under RT conditions, simulated with SHAW LE boundary conditions, may be a consequence of error in surface soil temperature propagated to calculations of soil surface vapor pressure by the SHAW module.

Differences in soil water dynamics calculated with LE passed from SHAW and PENFLUX modules could reflect structural differences in the modules. The SHAW module computes evaporative flux as the gradient in vapor pressure at the surface evaporative source and the ambient sink. The bias to drier soil conditions simulated with the SHAW module for RT conditions coincided with a bias to a warmer soil surface. These biases could be linked by propagation of positive bias in surface soil temperature to a positive bias in vapor pressure at the evaporative source of the soil surface. To illustrate, a relatively wet soil surface at 30 °C will have a vapor pressure of 4.24 kPa while a 35 °C surface will be at 5.62 kPa. The higher temperature creates a larger vapor gradient between the soil surface and the atmosphere, resulting in higher evaporation. Forcing these surface temperatures at noon on May 15 resulted in simulated evaporation of 0.55 and 0.68 mm/h, respectively. Increased evaporation will result in increased soil drying; drier soil will in turn result in less evaporative cooling at the surface, causing further surface temperature increase.

In contrast, PENFLUX uses the Penman (1948) approximation to quantify evaporative flux. As described in Monteith (1965), the combination equation for evaporative flux includes an enthalpy term (R_n–G)

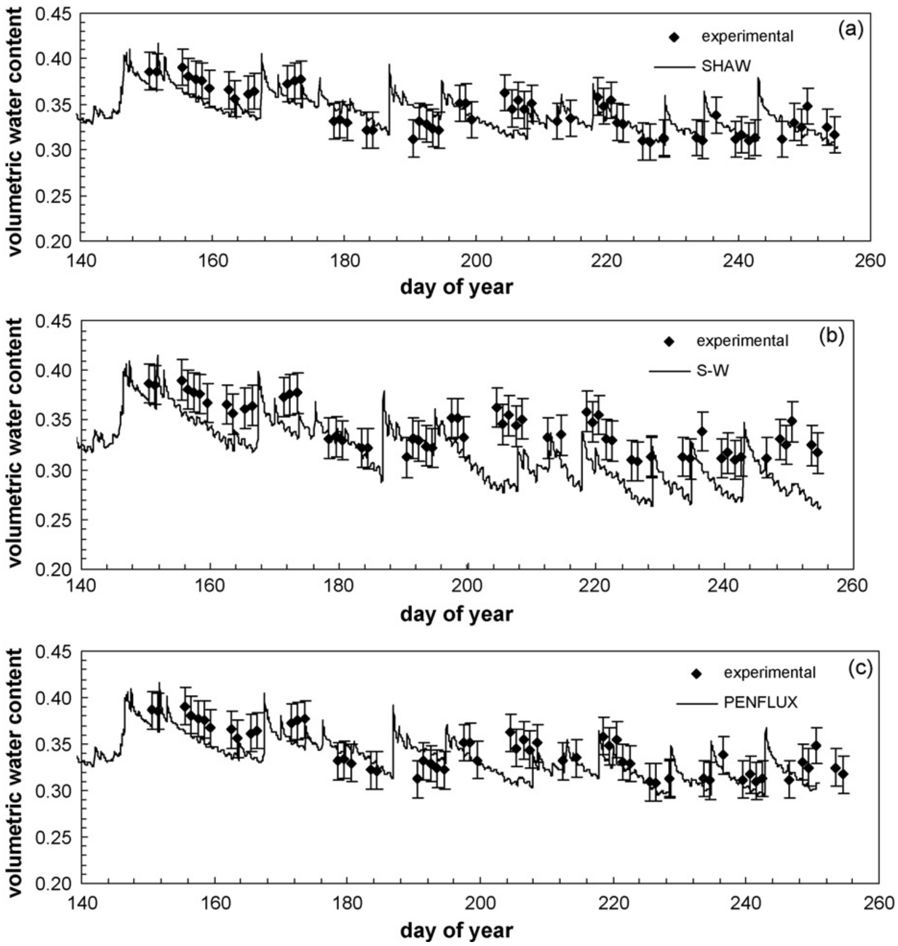

Fig. 8. Measured and simulated results of soil water content (0–30-cm interval, NT conditions) using RZ-SHAW modules (a) SHAW, (b) S–W, and (c) PENFLUX for May 6–September 10, 1996 (DOY 140–254).

representing absorbed energy, and an entropy term ($\delta e_s - \delta e_a$) representing gradients in vapor pressure deficits at the surface soil (δe_s) and reference ambient height (δe_a). In this case, biases in T_s are propagated to R_n, G, and δe_s terms. However, when the net short-wave radiation, R_{ns} is much greater than R_{nl}, these propagated errors are smaller in magnitude than errors propagated from biases in T_s for the gradient flux case. This effectively buffers calculations of LE from propagation of bias in surface boundary conditions under conditions of strong short-wave radiative loading.

Soil physical properties for each soil horizon were inferred from texture. Errors in specifying thermal and hydraulic properties propagate into errors in simulation output. Further, changes in surface residues can contribute to errors due to assumed constant residue conditions. Despite these probable system specification errors, systematic bias among modules permit analysis of likely conceptual problems.

SHAW and PENFLUX modules containing explicit solutions for surface temperature contributes sensitivity for residue effects on partitioning surface energy balance components. PENFLUX soil slab approximation likely contributes to trend in soil T and should be evaluated—particularly depth of slab and assumption of lower boundary temperature. In SHAW, near-surface aerodynamic and radiative transfer coefficients largely control energy partitioning; re-evaluation could provide improvements in predictive accuracy.

Results suggest that the greater detail afforded by the SHAW and PENFLUX modules in simulating the surface energy balance are more suitable for simulation of residue architecture effects on soil temperature and water dynamics. Strong soil–atmosphere thermal gradients under radiative loading and dry soil surface conditions preclude the isothermal assumption employed in this implementation of S–W. However, apparent mis-specification of near-surface energy exchange processes led to similar sets of biases for SHAW and PENFLUX modules in calculations of R_n and T_{s3} for conditions with and without surface crop residues.

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